

Figure 1

Applicant: Aranibar et al.

Serial No: Filed Concurrently Herewith

Thabolome Profiling Methods Using Chromatographic and Spectroscopic

It term Recognition Analysis

No. 16313-0089

Sheet 2 of 10

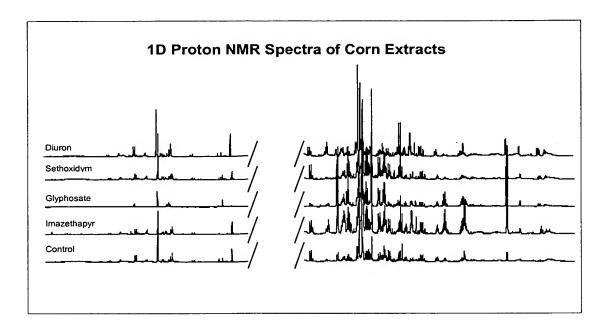


Figure 2

Applicant: Aranibar et al.	
Serial No: Filed Concurrently Herewith	
1etabolome Profiling Methods Using Chr	omatographic and Spectroscopi
attern Recognition Analysis	-
No. 16313-0089	Sheet 3 of 10

Training Set			Control	PURSUIT	Sethoxim	Glyphosate	Diuron	Foul	Assignment
na022400 02	2	Control	96666 0	c	0.00001	0.00003	0.00002	0.00001	Control
na022400_02	1 ע	o tro	0.00000	o C		00000	0.00003	00000	Control
200000000000000000000000000000000000000	, ĉ	Control	00000		o c	20000	00000	0000	Control
19000100_00	0 6		0.99990		<b>.</b>	0.0000	0.0000	20000	Control
ma030100_09	25.		0.93930	0	,	0.0000	0.000	0000	
na030100_11	4	PURSUIT	<b>o</b> '	0.99996	0.00001	0.00003	0.00004	0.00002	PURSON
na030100_14	37	PURSUIT	0	96666.0	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030100_17	6	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100 19	42	PURSUIT	0	0.99995	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030600 04	51	Control	0.99993	0	0.00002	0.00002	0.00001	0.00001	Control
na030600_08	55	Sethoxydim	0.00002	0.00001	96666 0	0.00005	0.00001	0.00004	Sethoxydim
na030600_10	2 2	Sethoxydim	00000	00000	0 99993	0 0000	00000	0 00004	Sethoxydim
na020600_13	5 6	Foul	2000	70000	00000			0 00001	Foul
100000	8 8	- C	0000	10000	0.0000			0000	Charbonato
11a05000_15	700	Glyphosale	00000	0.0000	00000	7666.0	> 0	0000	Clypinosate
nausubu_nb	3	Glypnosate	0.0000	0.0000	0.00003	0.88884	0	0.0000	Giyprosate
na030600_20	29	Dinron	0.00004	0.00004	0.00002	0	0.99993	0.00003	Diuron
na030600_21	89	Diuron	0.00007	0.00004	0.00002	0	0.99994	0.00003	Diuron
Toet Cot									
les sel				•	,	00000	00000	,0000	
na022400_01	<b>.</b>	Control	0.99998	9	0	0.00002	0.00003	0.0000	Contro
na022400_03	က	Control	96666.0	0	0.00001	0.0001	0.00002	0.00001	Control
na022400 04	4	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na022400_06	9	Control	0.99997	0	0.00002	0	0	0	Control
na022400_07		Control	0 99998		C	0 0000	0.00003	0.00001	Control
na022400_08	. α	Control	799990		0 0001	00001	0 0000	00000	Control
11a022400_00				0 00100		70000		90000	Introduct
na022400_03	ָר ת	PURSOIL		0.027.33	<b>.</b>	0.01224	> (	0.000	
na022400_10	9	PURSUIT	0.00086	0.00118	0	0.34361	0	0.00002	UNKHOWN
na022400_11	Ξ	PURSUIT	0.00085	0.00141	0	0.27197	0	0.00002	Unknown
na022400 12	12	PURSUIT	0.00016	0.0025	0	0.12513	0	0.00003	Unknown
na022400 13	13	PURSUIT	0.00013	0.00259	0	0.12979	0	0.00003	Unknown
na022400_14	4	PURSUIT	0.00013	0.00238	0	0.13242	0	0.00003	Unknown
na022400_15	15	PURSUIT	0	0.10029	0	0.00586	0.00001	0.0001	Unknown
na022400_16	16	PURSUIT	0.00005	0.00469	0	0.06222	0	0.00004	Unknown
na022400_17	17	TIIISAIIA	0.00114	0.00127		0 29608		0.0000	Unknown
n2022400 18	. α	TIIISAIIA	0.0004	0.00139		0 27092		0 0000	Unknown
na022400_10	5 6	PIDOID	9,000	0.00	• •	0.18002		00000	Ilnknown
114022400 13	<u>-</u> 6		0.000	5000	•	0.10332		0.0000	Lakaowa
na022400_20	8 3	ווויאסא	0.00214	0.00104	<b>-</b>	0.55051	> 0	0.0000	E CONTROLL
na022400_21	7	PURSUIT	0.00073	0.00088	0	0.34/62	<b>5</b>	0.00002	UNKNOWN
na022400_22	72	PURSUIT	0.00046	0.00146	0	0.25479	0	0.00002	Unknown
na022400 23	23	PURSUIT	0.00086	0.00123	0	0.3072	0	0.00002	Unknown
na030100_01	24	Control	96666.0	0	0	0.00002	0.00005	0.00001	Control
na030100_02	25	Control	0.99997	0	0	0.00001	0.00238	0.00001	Control
na030100_03	38	Control	79997	c	0	0.00001	0.0000	0.00001	Control
na030100 04	27	-	00000				0000		1
				_					

Figure 3a

pplicant:	Aranibar et al.	
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ata i	Recognition Analysis	•
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Halling Sec			Control	PURSUIT	Sethoxim	Glyphosate	Diuron	Foul	Assignment
na030100_07	စ္က	Control	0.99998	0	0	0.00002	0.00002	0.00001	Control
na030100 08	3	Control	0.99996	0	0.00002	0	0.00001	0.00001	Control
na030100_10	33	PURSUIT	0	0.99996	0.00001	0.00003	0.00005	0.00002	PURSUIT
na030100_12	32	PURSUIT	0	96666.0	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100_13	98	PURSUIT	0	96666.0	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100 15	జ္က	PURSUIT	0	0.99994	0.00003	0.00003	0.00005	0.00002	PURSUIT
na030100 16	33	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100_18	41	PURSUIT	0	0.99995	0.00002	0.00004	0.00004	0.00002	PURSUIT
na030100_20	43	PURSUIT	0	0.9999	0.00005	0.00003	0.00008	0.00003	PURSUIT
na030100_21	4	PURSUIT	0	0.99995	0.00004	0.00004	0.00003	0.00002	PURSUIT
na030100_22	45	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030600_12	ည	Sethoxydim	0.00005	0.0003	0.99701	0	0.00003	0.00003	Sethoxydim
na030600_14	61	Glyphosate	0.00006	0.00004	0.00002	0.99994	0	0.00003	Glyphosate
na030600 17	9	Glyphosate	0.00005	0.00005	0.00003	0.99993	0	0.00003	Glyphosate
na030600 18	65	Foul	0	0.00007	0.00003	0	0.00001	0.99993	Foul
na030600_19	99	Diuron	0.00034	0.00003	0.00002	0	0.99992	0.00003	Diuron
na030600_22	69	Diuron	0	0.00005	0.00003	0	0.99989	0.00004	Diuron
na030600_23	2	Diuron	0.00065	0.00014	0.00043	0	0.92715	0.00011	Dinron
na030600_24	7	Diuron	0.00002	0.00005	0.00003	0	0.99993	0.00003	Dinron
Training Set									
na022400_02	7	Control	0.99996	0	0.00001	0.00003	0.00002	0.00001	Control
na022400_05	2	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_06	53	Control	0.99998	0	0	0.00002	0.00003	0.00001	Control
na030100_09	33	Control	0.99998	0	0	0.00001	0.00004	0.00001	Control
na030100_11	怒	PURSUIT	0	96666.0	0.00001	0.00003	0.00004	0.00002	PURSUIT
na030100_14	37	PURSUIT	0	96666.0	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030100_17	숙	PURSUIT	0	0.99995	0.00002	0.00003	0.00004	0.00002	PURSUIT
na030100_19	45	PURSUIT	0	0.99995	0.00001	0.00004	0.00004	0.00002	PURSUIT
na030600 04	5	Control	0.99993	0	0.00002	0.00002	0.00001	0.00001	Control
na030600_08	22	Sethoxydim	0.00002	0.00001	0.99996	0.00005	0.00001	0.00004	Sethoxydim
na030600_10	24	Sethoxydim	0.00002	0.00002	0.99993	0.00002	0.00001	0.00004	Sethoxydim
na030600_13	9	Foul	0	0.00004	0.00002	0	0	0.99991	Foul
na030600_15	62	Glyphosate	0.00007	0.00004	0.00001	0.99992	0	0.00003	Glyphosate
na030600_16	83	Glyphosate	0.00006	0.00004	0.00003	0.99994	0	0.00003	Glyphosate
na030600_20	29	Diuron	0.00004	0.00004	0.00002	0	0.99993	0.00003	Diuron
na030600 21	89	Dinron	0.00007	0.00004	0.00002	0	0.99994	0.00003	Dinton

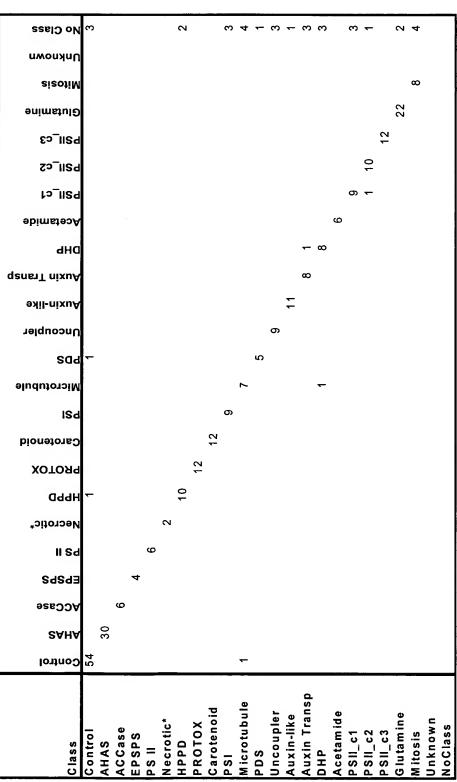
Figure 3b

SNNS result fil	е	V1.4-3D				
Training file		na022400				7
Test file na040	400					
No. of patterns	:	24				
No. of input un	its:	1080				
No. of output u	nits:	6				
Startpattern:		1				
Endpattern:		24				
Teaching output	included					
Treatment:	1.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99954	0.00045	0.00001	0.00001	0.00001	0.00001
Treatment:	2.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99936	0.00065	0.00001	0.00001	0.00001	0.00001
Treatment:	3.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99951	0.00047	0.00001	0.00001	0.00001	0.00001
Treatment:	4.1 Contro	1				
Target:	1	0	0	0	0	0
Output:	0.99963	0.00037	0.00001	0.00001	0.00001	0.00001
Treatment:	5.1 Chlors	ulfuron				
Target:	0	0	0	0	0	0
Output:	0.00159	0.99843	0	0.00001	0	0
Treatment:	6.1 Chlors	ulfuron				
Target:	0	0	0	0	0	0
Output:	0.00806	0.99165	0	0	0	0
Treatment:	7.1 Chlors	ulfuron				
Target:	0	0	0	0 .	0	0
Output:	0.00334	0.99669	0	0	0	0
Treatment:	8.1 Chlors	ulfuron				
Target:	0	0	0	0	0	0
Output:	0.00014	0.99985	0	0.00001	0	0
Treatment:	9.1 Chlors	ulfuron				
Target:	0	0	0	0	0	0
Output:	0.00667	0.99376	0	0	0	0
Treatment:	10.1 Imaza	methabenz				
Target:	0	0	0	0	0	0
Output:	0.00044	0.99955	0	0	0	0
Treatment:	11.1 Imaza	methabenz				
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	0	0	0	0
Treatment:	12.1 Imaza	methabenz				
Target:	0	0	0	0	0	0
Output:	0.00208	0.99798	0	0.00001	0.00001	0

Figure 4a

SNNS result fil	е	V1.4-3D				
Training file		na022400				
Test file na040	400					
No. of patterns	:	24				
No. of input un	its:	1080				
No. of output u		6				
Startpattern:		1				
Endpattern:		24				
Teaching output	included					
Treatment:	13.1 Imaza	methabenz		,		
Target:	0	0	0	0	0	0
Output:	0.00223	0.99755	0	0	0	0
Treatment:	14.1 Imaza	methabenz				
Target:	lo	0	0	0	0	0
Output:	0.06789	0.93484	0	0	0	0
Treatment:	15.1 Sulfu	meturon				
Target:	0	0	0	0	0	0
Output:	0.00046	0.99955	0	0	0	0
Treatment:	16.1 Sulfu	meturon				
Target:	0	0	0	0	0	0
Output:	0.00102	0.999	Ō	0.00001	Ō	Ō
Treatment:	17.1 Sulfu	meturon				
Target:	0	0	0	0	0	0
Output:	0.00194	0.99813	0	0.00001	0	0
Treatment:	18.1 Sulfu					
Target:	0	0	0	0	0	0
Output:	0.00013	0.99987	0	0	0	0
Treatment:	19.1 Sulfu	meturon				
Target:	lo	0	0	0	0	0
Output:	0.00014	0.99985	0	0	0	0
Treatment:	20.1 Imaza	pvr		<del>(20. )(20. )</del>		
Target:	0	0	0	0	0	0
Output:	0.0018	0.998	0	0	0	0
Treatment:	21.1 Imaza	pyr				
Target:	0	0	0	0	0	0
Output:	0.00031	0.99968	0	0.00001	0	0
Treatment:	22.1 Imaza	pvr				
Target:	0	0	0	0	0	0
Output:	0.00175	0.99791	0	0	0	0
Treatment:	23.1 Imaza					
Target:	0	0	0	0	0	0
Output:	0.00018	0.9998	Ō	0	0	0
Treatment:	24.1 Imaza					
Target:	0	0	0	0	0	0
Output:	0.06579	0.93074	0	0	Ö	0
F		<del>.</del>		-	-	

Figure 4b



Applicant: Aranibar et al.
Serial No: Filed Concurrently Herewith

tabolome Profiling Methods Using Chromatographic and Spectroscopic ktern Recognition Analysis o. 16313-0089 Sheet 7 of 10

Rows: Teaching Input; Columns: Classification for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 5

Applicant: Aranibar et al.

Serial No: Filed Concurrently Herewith
etabolome Profiling Methods Using Chromatographic and Spectroscopic
httern Recognition Analysis

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	_	_				_		_				_		,			_	,				,	,	
# Plants	31	17	2	7	0	-	9	9	9	9	9	3	9	9	9	9	т	9	2	9	12	9	0	0
Ппкпочп	7	0	0	0	0	0	m	0	0	7	4	7	_	7	7	5	-	7	-	0	0	3	0	0
Spare	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SisosiM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0
Glutamine	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Ξ	0	0	0
PSII_e3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0
PSII_c2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-	∞	0	0	0	0	0
PSII_c1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	-	0	0	0	0	0
Acetamide	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0	0	0	0
онь	0	0	0	0	0	0	0	0	0	0	0	0	-	0	-	-	0	0	0	0	0	0	0	0
qenerT nixuA	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0
Auxin-like	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0
Quconbjer	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0
PDS	1	0	0	0	0	0	0	0	0	0	0	-	0	0	0	0	0	0	0	0	0	0	0	0
Microtubule	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ISA	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Carotenoid	0	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
хотояч	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
НРРБ	1	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Necrotic*	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Not Used	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
EPSPS	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98£⊃⊃A	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SAHA	0	17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Control	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
CLASS	Control	AHAS	ACCase	EPSPS	Not Used	Necrotic*	ПРР	PROTOX	Carotenoid	ISd	Microtubule	SQA	Uncoupler	Auxin-like	Auxin Transp	DHP	Acetamide	PSII_c1	73_IISA	to_IISA	Glutamine	Mitosis	Spare	NoClass

Rows: Teaching Input; Columns: Classifications for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)

Figure 6

SAHA

Control

100

Control AHAS

MOA

		Titl Da Doc	1	olom n Re 1631:	cogn	utic	ing I	Meti naly	hod: sis	Us	ing	Chr	omai	logr			d Sp		osco	pic
Nukuown	5.8				17			25	33	17	25	8.3	25	25		25	8.3		8.3	33
Spare																				
Mitosis																				67
Glutamine																			92	
เว_แล <b>ฯ</b>																		100		
รอไเรส																	83			١
<b>เว</b> าแรง																75	œ			
Acetamide .															100					
ОНЬ													æ	29						
qensıT nixuA													29							
Auxin-Ilke												92								
Nuconblet											75									
PDS	7									83										
Microtubule									58					œ						
ISA								7.5												
Carotenoid							100													
хотояч						100														
Оччн	7				83															
Necrotic*				100																
II Sd			100	•																
EPSPS		9	001																	
essOOA		100	_																	
925DA	l	7																		

8

Microtubule P D S

Carotenoid PSI

Necrotic\* HPPD PROTOX

ACCase EPSPS PS II

Uncoupler Auxin-like Auxin Transp DHP

Necrotic = dead or decaying plant Mitosis

Acetamide PSII\_c1 PSII\_c2 PSII\_c3 Glutamine

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, 1 "Spare" Class, and "Unknown" Added by SNNS)



Ппкпоwn	9		Γ				20	Γ		33	29	29	17	33	33	83	33	33	2			20
Spare	-			T							$\vdash$		$\top$	T				†		-	$\dagger$	<del>                                     </del>
sisotiM												1					<del>                                     </del>		1	T		20
Glutamine														-							32	T
E5_1129																				8		
PSII_c2							Г											17	∞			
12_112¶		Ī																20	2			
9bimat99A																	19					<u> </u>
													17		17	17						
qenerT nixuA															20							
Auxin-like														29								
Uncoupler													29									
Saq	3											33										
Microtubule											33											
ISd										29												
Carotenoid									100													
хотояч								100														
нььр	<u>س</u>						20															
Necrotic*						100																
Not Used																						
EPSPS				8																		
ACCase			100																			
SAHA		100																				
Control	83																				8	
Class	<u></u>	-	7	6	4	5	9	7	∞	6	10		12		4	15	16	11	18	19	20	21
CLASS	Control	AHAS	ACCase	EPSPS	Not Used	Necrotic*	HPPD	PROTOX	Carotenoid	PSI	Microtubule	PDS	Uncoupler	Auxin-like	Auxin	DHP	Acetamide	PSII_c1	PSII_c2	PSII_c3	Glutamine	Mitosis

Rows: Teaching Input, Columns: Classification as Percentage of Total Plants Tested for Nineteen MOAs (23 Classes, Including "Control" = Untreated Plants, I "Spare" Class, and "Unknown" Added by SNNS)

Figure 8